

A MULTI-TEMPERATURE MODEL OF SHOCK STRUCTURE FOR AEROTHERMODYNAMIC CALCULATION

Chunpei Cai Danny D. Liu
ZONA Technology Inc.

Kun Xu
The Hong Kong University of Science and Technology

ABSTRACT

Accurately computing the inner structure of normal shock waves or oblique shock waves is crucial for many hypersonic applications. As such, it will improve the prediction accuracy of aerodynamics properties and aerothermal effects on hypersonic vehicles and spacecrafts during atmospheric entries. Because a shock wave usually has a thickness of a few mean free paths, it is quite difficult to accurately compute the detailed non-equilibrium inner structure across a shock wave with a continuum method.

In this paper, we report our recent progress in developing a Gas-kinetic Bhatnagar-Gross-Krook (BGK) scheme for computations of one-dimensional, vibrational, non-equilibrium nitrogen flows through a planar shock wave. The present Gaskinetic-BGK scheme is a generalization of the work of Xu,^{1,2} in that it solves for the shock structure with multiple temperatures, including two translational temperatures, one rotational temperature and one vibrational temperature. The salient features of the present Gaskinetic-BGK method are multi-fold. Its applicability covers a wide simulation regime extending that of continuum flows to the transition flows; it is more computational efficient than the traditional direct simulation Monte Carlo (DSMC) method³ in time for shock wave simulation; it does not require additional or special techniques to stabilize the shock wave. To provide proper downstream subsonic boundary conditions for very strong shock waves, it is required to determine a proper post-shock equilibrium state where all temperatures have complete relaxation processes to a common equilibrium temperature. Analytical expressions of a complete set of generalized Rankine-Hugoniot Relations across a planar shock wave are obtained to account for the variant specific heat ratio γ due to inner energy excitations. Numerical simulation results by the present Gaskinetic-BGK method and the DSMC method are found in good agreement.

INTRODUCTION

Hypersonic rarefied gasdynamics for practical aerothermodynamic consideration often lies in the transition regime where the Knudsen number range is of order 0.01~0.1. In this regime, hypersonic rarefied air flows are characterized by large non-equilibrium regions with multiple temperatures, including different translational temperature T_n , T_t , rotational temperature T_r and vibrational temperature T_v . There have been several approaches that attempted to solve this

problem. DSMC can easily model the non-equilibrium physics but it becomes increasingly expensive as the Knudsen number gets closer to the lower end of the transition region. On the other hand, classical continuum solution using Computational Fluid Dynamics (CFD) is found to deteriorate as the flow is approaching this transition regime. Directly solving the Boltzmann equation by retaining the complete collision integral is hampered by the difficulty in the incorporation of the non-equilibrium physics and the extremely expensive simulation cost.

The BGK model of the Boltzmann equation appears to provide a viable method to solve for the non-equilibrium flow problem because of its ease of formulation in the multi-temperature modeling of the distribution functions. But mostly the current BGK approaches are confined to flows of low Mach number. Among them the BGK-Xu method stands out as a promising approach to compute for hypersonic non-equilibrium flows with shock waves. The outstanding features of the BGK-Xu method are described in a review paper of Xu⁴.

The major part of the present work is an improvement of the BGK-Xu model in that it is based on Xu's earlier work in References 1, 2. We proposed a complete BGK model prior to flow dissociation for the computation of a one-dimensional shock wave with all possible multiple temperatures, namely, two translational temperatures T_n , T_t , one rotational temperature T_r , and one vibrational temperature T_v . To validate this new scheme, a test case of $M_\infty=10.0$ is simulated with the BGK scheme and the DSMC method. For both the BGK scheme and the DSMC method, proper downstream equilibrium boundary conditions are required for the simulation. However, due to the consideration of the vibrational energy, the specific heat ratio $\gamma=C_p/C_v$, is variant across the shock waves. Hence, the classical Rankine-Hugoniot relations are not applicable. In this study, we derived a set of generalized Rankine-Hugoniot relations, with them the proper downstream flow conditions can be determined for the DSMC and BGK simulations.

A ONE-DIMENSIONAL MULTIPLE-TEMPERATURE BGK MODEL

In this section, we propose a general one-dimensional kinetic BGK scheme to compute non-equilibrium flows with multiple temperatures. The model is applicable in simulations of planar shock waves with monatomic, diatomic and polyatomic molecules.

The Boltzmann equation expresses the behavior of a many-particle kinetic system in terms of the valuation equation for a single particle gas distribution function. The right hand side of the Boltzmann, which is mainly two body collisions, are valid in a large range from several hundreds of atmosphere to free molecular flow.⁵ To simplify the Boltzmann equation, the BGK model is formulated as

$$\frac{\partial f}{\partial t} + u \frac{\partial f}{\partial x} = \frac{g - f}{\tau} \quad (1)$$

where f is the normalized number density distribution of molecules at position, and particle velocity u , at time t . For the right hand side term, $\tau = \mu/p$, is the characteristic relaxation time,

and μ can be computed by the Surtherland's law; g is the equilibrium state of gas with the following specific expression:

$$g = \rho \left(\frac{\lambda_x}{\pi}\right)^{1/2} \exp(-\lambda_x(u-U)^2) \left(\frac{\lambda_t}{\pi}\right)^{K_t/2} \exp(-\lambda_t \xi_t^2) \left(\frac{\lambda_r}{\pi}\right)^{K_r/2} \exp(-\lambda_r \xi_r^2) \left(\frac{\lambda_v}{\pi}\right)^{K_v/2} \exp(-\lambda_v \xi_v^2) \quad (2)$$

where ρ is the density, U is the macroscopic fluid velocity along the x-direction, $\lambda = m/(2kT)$, m is the molecular mass, k the Boltzmann constant, and T is a specific temperature. For an equilibrium flow, the internal variable ξ accounts for the tangential, rotational and vibrational modes, and has an expression of $\xi^2 = \xi_t^2 + \xi_r^2 + \xi_v^2$, in which ξ_t , ξ_r , ξ_v have K_t , K_r and K_v degrees of freedom of translational, rotational, and vibration energy. For nitrogen, $K_t = 2, K_r = 2$, while K_v is decided by the vibrational energy, Eqn.(19). Notice the specific heat ratio γ is not constant for vibrational non-equilibrium flow, and must be computed locally in each time step for each cell:

$$\gamma = \frac{3 + K_r + K_v + 2}{3 + K_r + K_v} \quad (3)$$

The mass ρ , momentum ρU , total energy ρE , thermal energy along the tangential direction ρE_t , rotational energy ρE_r , and vibrational energy ρE_v , are the moments of f :

$$W = (\rho, \rho U, \rho E, \rho E_t, \rho E_r, \rho E_v)^T = \int \Psi f dud\xi_t d\xi_r d\xi_v \quad (4)$$

where Ψ has the components

$$\Psi = (1, u, \frac{1}{2}(u^2 + \xi_t^2 + \xi_r^2 + \xi_v^2), \frac{1}{2}\xi_t^2, \frac{1}{2}\xi_r^2, \frac{1}{2}\xi_v^2)^T \quad (5)$$

and the volume element in the phase space with $dud\xi = dud\xi_t d\xi_r d\xi_v$. Since only mass, momentum, and total energy are conserved during particle collisions, the collision term on the right hand side of the BGK model equation satisfies the following collision condition:

$$\int (g - f) \psi_\alpha dud\xi_t d\xi_r d\xi_v = S = (0, 0, 0, s_t, s_r, s_v)^T \quad (6)$$

where $\alpha = 1, 2, 3, 4, 5, 6$, the source terms are modeled as $s_t = \rho R(T_t - 0.5(T_{tr} + T_{tr,r}))/\tau$, $s_r = \rho R(T_r - T_{tr})/(Z_r \tau)$, $s_v = \rho(RT_{vib} - e_v(T_{tr}))/ (Z_v \tau)$, T_t , T_r , T_v , T_{tr} and $T_{tr,r}$ are instantaneous temperatures along, normal to the shock plane, internal rotational, vibrational, averaged translational, and averaged translational and rotational temperatures, respectively. Z_r and Z_v are the relaxation parameters for rotational and vibrational temperature. Notice in this scheme, we assume that the rotational and vibrational temperatures relax towards the equilibrium translational temperature, based on the consideration that the internal energy is obtained through exchanges of energy from the translational energy.

Base on the above BGK model, the Navier-Stokes equations can be derived with the Chapman-Enskog expansion with the 1st-order expression only:

$$f = g - \tau(\partial g / \partial t + u \partial g / \partial x) \quad (7)$$

To provide the gradients, in the expression for g, ρ, U, λ are assumed to be functions of both time and space. ⁴The process to calculate the slope in the equilibrium distribution g in Equation 7 is quite complex, and the final format is appended at the end of this paper. Note the solutions in the appendix are a general set of solutions, which are applicable to other situations such as monatomic flows by forcing the coefficients a_5 and a_6 to be zero. They are also applicable to study the rotational temperature relaxation-only process by setting a_6 to zero.

In order to validate the above model, a finite volume method is used to solve the BGK model:

$$W_j^{n+1} = W_j^n + \frac{1}{\Delta x} \int_0^{\delta t} [F_{j-1/2}(t) - F_{j+1/2}(t)] dt + S_j^n \delta t \quad (8)$$

where W_j^n is the cell-averaged mass, momentum, total energy, thermal energy in tangential direction, rotational energy, and vibrational energy. $F_{j+1/2}$ is the corresponding fluxes at a cell interface by solving the Boltzmann equation. In this scheme, the flux is calculated by the following format:

$$F = \int u \Psi(f + f_{eq}) / 2 du d\xi_t d\xi_r d\xi_v \quad (9)$$

Note that δt is the time step $\delta t = t^{n+1} - t^n$, and S_j^n is the source term in the thermal energy equation. The evaluation of the fluxes is based on the gas distribution function f and f_{eq} at a cell interface, while the f is a multiple temperature distribution function and f_{eq} is a one temperature equilibrium distribution function. The evaluation of flux by averaging with an equilibrium state velocity distribution function f_{eq} is helpful to obtain a reasonable density profile across strong shock waves. In the flux evaluations, the Prandtl number fix⁴ is applied for all the energy fluxes.

For strong shock wave computation, the specific relaxation time τ must consider gradient term. For this purpose, a generalized collision time τ_* is introduced in the numerical scheme, its relation to the collision time τ ,⁶ which is well-defined in the continuum flow regime:

$$\tau_* = \frac{\tau}{1 + \tau(D^2 f^{eq} / Df^{eq})} \quad (10)$$

GENERALIZED RANKINE-HUGONIOT RELATIONS: TO DETERMINE POST STRONG SHOCK EQUILIBRIUM STATE

In order to test the above multiple temperature BGK scheme with simulations of the inner structures of planner shock waves, one natural requirement is to specify a post-shock equilibrium state as proper downstream boundary conditions. Due to the fact that the downstream flow is always subsonic, the accuracy of the downstream boundary conditions have significant effects on the simulation.

For monatomic molecular gas, there is no vibrational and rotational temperature, and the specific heat ratio, $\gamma = C_p/C_v$, maintains a constant through shock waves, as long as the post-shock temperature is not high enough to trigger the ionization process. Hence, the classical Rankine-Hugoniot relation can provide the boundary conditions. However, for diatomic or polyatomic molecules, because of the vibrational degree of freedom will be activated under high temperature, the specific heat ratio, γ , will be variant across the shock wave. For this reason, we first proceed to obtain general formulations to decide the post-shock equilibrium state for diatomic or polyatomic molecule gas. At this equilibrium post-shock state, we assume all temperature relaxation process has complete and the post-shock equilibrium temperature is not strong to trigger severe dissociation.

For a planar shock wave, the control equations of density, momentum and energy equations are:⁷

$$\frac{d}{dx}(\rho u) = 0 \quad (11)$$

$$\frac{d}{dx}(p + \rho u^2 - \frac{4}{3}\mu \frac{du}{dx}) = 0 \quad (12)$$

$$\frac{d}{dx}[\rho u(\frac{\gamma}{\gamma-1}RT + \frac{u^2}{2}) - \frac{4}{3}\mu u \frac{du}{dx} - \kappa \frac{dT}{dx}] = 0 \quad (13)$$

Select a one-dimensional control volume with one side in the pre-shock region and another side in the post-shock equilibrium region. The length of this control volume can be sufficiently long to reach the post-shock equilibrium state. Denote the pre-shock state as state “1”, and the post-shock state, where all thermal relaxations are complete, as state “2”. For these two equilibrium states, we can assume that both satisfy thermally perfect assumption that $p = \rho RT$, where $R_1 = R_2$. Hence, no dissociation effect should happen. Notice for both states, all gradients are zero, hence, after several steps of derivations, simple relations between these two states can be obtained as followings:

$$\frac{T_2}{T_1} = \frac{\frac{\gamma_1}{\gamma_1-1} + \frac{\gamma_1}{2}M_1^2}{\frac{\gamma_2}{\gamma_2-1} + \frac{\gamma_2}{2}M_2^2} \quad (14)$$

$$\frac{u_2}{u_1} = \sqrt{\frac{\gamma_2}{\gamma_1}} \frac{M_2}{M_1} \sqrt{\frac{\frac{\gamma_1}{\gamma_1-1} + \frac{\gamma_1}{2}M_1^2}{\frac{\gamma_2}{\gamma_2-1} + \frac{\gamma_2}{2}M_2^2}} \quad (15)$$

$$\frac{p_2}{p_1} = \frac{1 + \gamma_1 M_1^2}{1 + \gamma_2 M_2^2} \quad (16)$$

$$\frac{(1 + \gamma_1 M_1^2)^2}{(\frac{\gamma_1}{\gamma_1-1} + \frac{\gamma_1}{2}M_1^2)\gamma_1 M_1^2} = \frac{(1 + \gamma_2 M_2^2)^2}{(\frac{\gamma_2}{\gamma_2-1} + \frac{\gamma_2}{2}M_2^2)\gamma_2 M_2^2} \quad (17)$$

The derivation process is similar to that for the classical Rankine-Hugoniot relation, which can be found in many textbooks, such as the book by Saad.⁸ However, to our surprise, we did not find

any article in the literature reported the above equations, which links the two states with variable specific ratio γ . We call the above equations generalized Rankine-Hugoniot Relations across shock waves. The most related previous results can trace back to Tisen⁹ and Egger¹⁰, they have studied the real gas effects in hypersonic flows by considering Van Der Waal's equation of state or the Berthelot's equation of state. Due to the relative compactness and general application scope, the generalized Rankine-Hugoniot Relations can be considered between the classic shock waves relations without real gas effects and the results by Tsien and Eddgar. The significance of the above relations is, for equilibrium flows across a shock wave, where relaxation process are assumed to be very fast, the above equations provide a set of post shock state calculation formula; to compute the inner relaxation process across the shock waves with finite relaxation speed, the above equations provide proper downstream boundary conditions.

Though the above equations explicitly list the post-shock Mach number and specific heat ratio γ , to solve the above equation, we need to provide the expression for the specific heat ratio γ as the necessary condition to solve out the post-shock state Mach number. To consider the vibrational effects for diatomic molecules with the simple harmonic oscillator model, the specific vibrational energy associated with a mode having a characteristic vibrational temperature Θ_v is:⁴

$$e_v = \frac{R\Theta_v}{\exp(\Theta_v/T) - 1} \quad (18)$$

The effective number of degrees of freedom at temperature T is:

$$K_v = \frac{2\Theta_v/T}{\exp(\Theta_v/T) - 1} \quad (19)$$

For diatomic molecule and linear polyatomic molecule, the rotational degree is $K_r=2$, while for nonlinear polyatomic molecule, the rotational degree of freedom is $K_r=3$. Then the following iteration process is clear: First with a specific γ , use Equation (17) to decide an intermediate post-shock Mach number M_2 ; Second, use this Mach number M_2 to decide a post-shock temperature T_2 with Equation (14); Third, use Equations (18, 19, 3) to decide a new specific heat ratio γ_2 . The above three steps proceed until a tolerance is reached.

Discussions

1. The above generalized Rankine-Hugoniot Relations consider vibrational temperature effects, and are applicable in a wider range of temperature. If the post-shock temperature is quite close or higher than dissociation temperature, then they are not applicable. If γ_2 is set to γ_1 , then the above relations consistently degenerate to the classical Rankin-Hughonit relations across planar shock waves.

2. For hypersonic limit case, i.e., the incoming Mach number is significantly large, $M_1 \rightarrow \infty$, then $M_2 \rightarrow \sqrt{\frac{\gamma_2-1}{2\gamma_2}}$, and $\frac{\rho_1}{\rho_2} = \frac{u_2}{u_1} \rightarrow \frac{\gamma_2-1}{\gamma_2+1}$, $\frac{T_2}{T_1} \rightarrow \frac{\gamma_2-1}{\gamma_2+1} \frac{p_2}{p_1}$. These relations are still compatible with the

classical results under hypersonic limit, but it is interesting to notice that the post-shock equilibrium state has no relations with γ_1 , i.e. the pre-shock factor γ_1 are forgot.

3. Figure 1 shows two profiles of post-shock Mach number with and without this variant specific heat ratio approaches. For the constant specific heat ratio case, the specific heat ratio value is set to $\gamma=1.4$. The incoming flow parameters are $T_\infty = 300K$, $P_\infty = 1.10325 \times 10^5 Pa$, and the gas is nitrogen. The post-shock Mach number with constant specific heat ratio is included. Figure 2 shows the post-shock equilibrium state pressure and temperature results vs. different incoming Mach numbers, with $T_\infty = 300K$ and $p_\infty = 1.01325 \times 10^5$. It is evident that, with the consideration of vibrational temperature, or a variant γ case, the post-shock equilibrium temperature is lower than the case of constant γ , while the pressure is higher. Hence, the difference in density is well announced for hypersonic flow with or without vibrational energy effect.

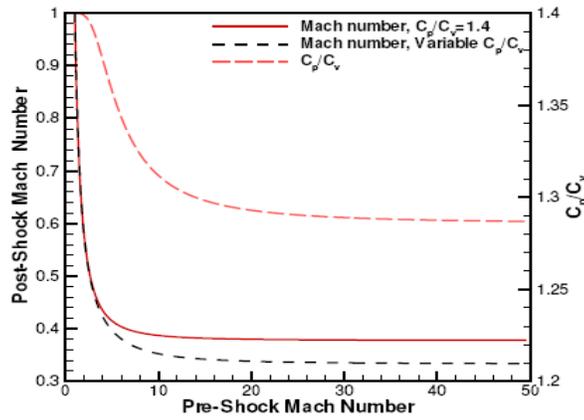


Figure 1. Profiles of post shock Mach number, and specific heat ratio. (N_2 , $T_\infty = 300 K$, $\rho_\infty = 1.01325 \times 10^5 Pa$)

4. The derivation process assumes $p = \rho RT$, and the same R are used in the pre-shock and post-shock regions. Hence, when the post-shock temperature is close to the characteristic dissociation temperature Θ_d , the solution is not applicable because R is not constant. We can use this dissociation temperature to estimate the asymptote values:

$$K_v \rightarrow \frac{2\Theta_v/\Theta_d}{\exp(\Theta_v/\Theta_d) - 1} \approx \frac{4}{2 + \Theta_v/\Theta_d}, \gamma \rightarrow \frac{18 + 7\Theta_v/\Theta_d}{14 + 5\Theta_v/\Theta_d} \quad (20)$$

The above approximation uses the fact that the characteristic vibrational temperature is far less than the dissociation temperature $\Theta_v \ll \Theta_d$. The asymptotic solution for the post-shock Mach number is:

$$M_2 \rightarrow \sqrt{\frac{\gamma_2 - 1}{2\gamma_2}} = \sqrt{\frac{2\Theta_d + \Theta_v}{18\Theta_d + 7\Theta_v}} \rightarrow \frac{1}{3} \quad (21)$$

This limit value is smaller than the constant specific heat ratio, which is $\sqrt{1/7}$ for nitrogen. The physical reason for this 11% lower value of post-shock Mach number for gas nitrogen is

obvious: with the consideration of the vibrational temperature, which has the significantly wider energy level, more post-shock energy are transferred more into the thermal energy, hence, the kinetic energy, is significantly lower than the kinetic energy without a consideration of the vibrational effect.

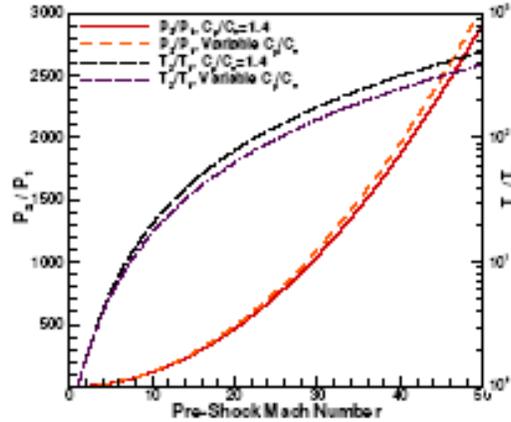


Figure 2. Profiles of post shock Pressure and Temperatures. (N_2 , $T_\infty = 300 \text{ K}$, $\rho_\infty = 1.01325 \times 10^5 \text{ Pa}$)

NUMERICAL SIMULATION AND DISCUSSION OF RESULTS

We implemented the above GasKinetic BGK scheme and performed one numerical simulation of a strong planar shock wave with $M=10.0$. In this simulation, the specific relaxation number Zr and Zv are set to 3 and 50, correspondingly. To compare the results, a DSMC simulation is performed for the same case as well by using a DSMC package named MONACO¹¹, developed at the University of Michigan.

To properly use the generalized Rankine-Hugoniot relations, in the simulation, we adopted a long simulation domain where the downstream boundary is 5 times of the shock thickness.

To accelerate the simulations, for both the BG and the DSMC simulations, the computational field are initialized with step profiles, where the post-shock quantities are obtained with our generalized Rankine-Hugoniot Relations instead of common Rankin-Hugoniot relations. The BGK scheme used $\partial()/\partial x = 0$ boundary conditions to compute the flux from the downstream boundary, and the specific heat ratio γ is recalculated at each time step and for each cell. In the DSMC simulation, the moving piston scheme⁴ at the downstream boundary is used, and a standard shock stablization process⁴ is adopted in the simulation as well. In all the simulations, the gas is assumed to be nitrogen, though the current BGK package can be used to simulate shock waves with monatomic gas. In the following results, density and temperature profiles are normalized by the values at both sides of the shocks, for example, $T = (T - T_{pre}) / (T_{post} - T_{pre})$. In

the BGK simulation, the viscosity is using the following formula: $\mu = 1.656 \times 10^{-5} \left(\frac{T}{273}\right)^{0.74}$.

Correspondingly, the Variable Hard Sphere (VHS) model was used in the DSMC simulation with index factor $\omega=0.74$.

In the DSMC simulation, the translational-vibrational energy exchanges are set to happen with a probability of 0.02. To be consistent with the relaxation rate in the MONACO package, we adopted $Z_r = 3.0$ and $Z_v = 50.0$ in the BGK simulation. We want to point out that it is very difficult for the BGK scheme to repeat the exact energy re-distribution relations in the DSMC method, when the vibrational energy relaxation is evolved.

To illustrate the vibrational effects, we choose a case with strong shock waves. The computation parameters are as followings: $M_\infty = 10.0$, $T_\infty = 226.149$ K, $\rho_\infty = 1.7413 \times 10^{-2} \text{ kg/m}^3$. For this case, the thermal non-equilibrium effect is significant and the equilibrium specific heat ratio are $\gamma_1 = 1.399$ and $\gamma_2 = 1.3193$, correspondingly.

Figure 3 shows preliminary number density profiles; Figure 4 shows the two translational temperatures and Figure 5 shows the rotational, vibrational temperature profiles and the specific heat ratio profiles. It is quite evident that the thermal non-equilibrium effects and the relaxation processes are clearly captured. Better matches can be obtained by changing the relaxation factor Z_r and Z_{vib} , however, to compare the results between the BGK and the DSMC results, we fixed these two numbers. We must also point it out that due to some difference associated with these two methods, especially when considering the vibrational effects, it is very difficult to achieve accurate match between these results. And it is also worthy to mention that, we did not find any previous publications in the literature reporting any similar DSMC simulations and BGK simulations.

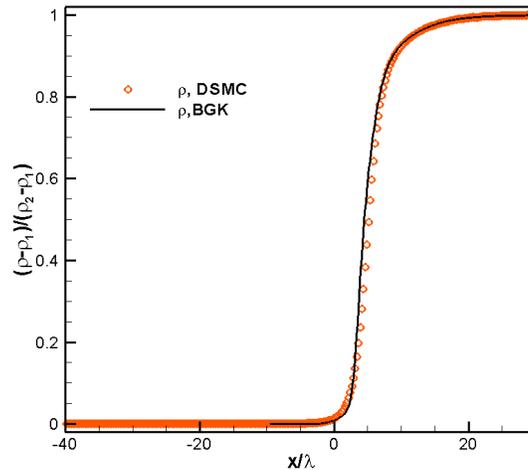


Figure 3. Profiles of density in an M=10 nitrogen shock wave. (BGK result, $T_\infty = 226.649$ K, $\rho_\infty = 1.741315 \times 10^{-3} \text{ kg/m}^3$)

We want to point out that though the BGK scheme development is complete, the current results are just preliminary. Both the BKG scheme results and the DSMC results will be improved and with more comprehensive test cases will be included in a future paper.

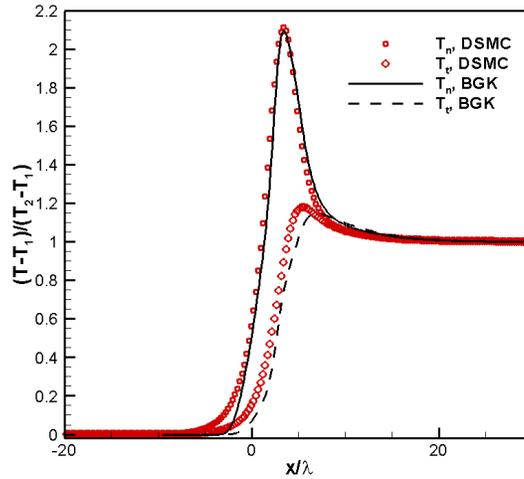


Figure 4. Profiles of translational temperatures in an M=10 nitrogen shock wave.(BGK result, $\rho_\infty = 1.741315 \times 10^{-3} \text{ kg/m}^3$, $T_\infty = 226.649 \text{ K}$)

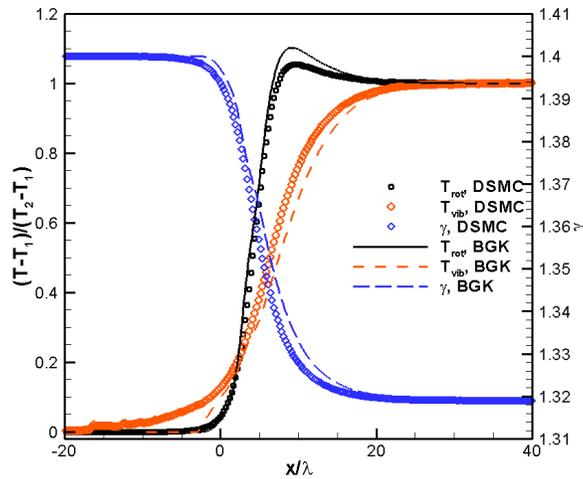


Figure 5. Profiles of rotational, vibrational temperatures and γ in an M=10 nitrogen shock wave.(BGK result, $\rho_\infty = 1.741315 \times 10^{-3} \text{ kg/m}^3$, $T_\infty = 226.649 \text{ K}$)

CONCLUSIONS

In this paper, we reported our recent progress in developing a 1D thermal nonequilibrium GasKinetic BGK solver. This BGK solver considered vibrational energy effects, and can be used in simulating the inner structures of strong shock waves. Compared with the DSMC method, this scheme is capable of reducing the simulation cost. Another merit of this scheme is that the shock wave is stable during the computation. Hence, no special stabilization treatment as the DSMC method required, are needed. During the numerical simulation of shock waves, to provide proper downstream boundary conditions at equilibrium state, a set of generalized Rankine-Hugoniot relations are obtained, and used to provide the downstream boundary

conditions for both the DSMC method and the BGK schemes. Numerical simulations of strong shock waves indicate that the BGK schemes can capture the inner structures for the shock waves with vibrational energy effects.

This development sets a solid foundation for the future constructions of general two-dimensional and three-dimensional GasKinetic BGK schemes for thermal non-equilibrium flows.

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APPENDIX

The equilibrium state of gas is:

$$g = \rho \left(\frac{\lambda_x}{\pi}\right)^{1/2} \exp(-\lambda_x(u-U)^2) \left(\frac{\lambda_t}{\pi}\right)^{K_t/2} \exp(-\lambda_t \xi_t^2) \left(\frac{\lambda_r}{\pi}\right)^{K_r/2} \exp(-\lambda_r \xi_r^2) \left(\frac{\lambda_v}{\pi}\right)^{K_v/2} \exp(-\lambda_v \xi_v^2) \quad (22)$$

where ξ_t , ξ_r , ξ_v have K_t , K_r and K_v degree of freedom of translational, rotational, and vibration energy. Since

$$(\rho, \rho U, \rho E, \rho E_t, \rho E_r, \rho E_v)^T = \int g \psi d\Phi \quad (23)$$

where ρE , ρE_t , ρE_r and ρE_v are the total, translational, rotational and vibration energy, correspondingly, and $\psi = \{1, u, \frac{1}{2}(u^2 + \xi_t^2 + \xi_r^2 + \xi_v^2), \frac{1}{2}\xi_t^2, \frac{1}{2}\xi_r^2, \frac{1}{2}\xi_v^2\}$.

By the Taylor expansion,

$$\frac{\partial g}{\partial x} = (a_1 + a_2 u + a_3 u^2 + a_4 \xi_t^2 + a_5 \xi_r^2 + a_6 \xi_v^2) g \quad (24)$$

and

$$\frac{\partial}{\partial x} (\rho, \rho U, \rho E, \rho E_t, \rho E_r, \rho E_v)^T = \int \frac{\partial g}{\partial x} \psi d\Phi \quad (25)$$

where $d\Phi = du d\xi_t d\xi_r d\xi_v$.

The above equations have the following solutions:

$$a_6 = \frac{4\lambda_v^2}{K_v} \frac{\partial(\rho E_v)}{\rho \partial x} - \frac{\partial \rho}{\rho \partial x} \lambda_v, \quad a_5 = \frac{4\lambda_r^2}{K_r} \frac{\partial(\rho E_r)}{\rho \partial x} - \frac{\partial \rho}{\rho \partial x} \lambda_r, \quad a_4 = \frac{4\lambda_t^2}{K_t} \frac{\partial(\rho E_t)}{\rho \partial x} - \frac{\partial \rho}{\rho \partial x} \lambda_t \quad (26)$$

Then, define

$$A = \frac{\partial \rho}{\rho \partial x} - \frac{K_v}{2\lambda_v} \frac{\partial(\rho E_t)}{\rho \partial x} - \frac{K_r}{2\lambda_r} \frac{\partial(\rho E_r)}{\rho \partial x} - \frac{K_t}{2\lambda_t} \frac{\partial(\rho E_v)}{\rho \partial x}, \quad B = \frac{\partial(\rho U)}{\rho \partial x} - \frac{\partial \rho}{\rho \partial x} U \quad (27)$$

$$C = \frac{\partial(\rho E)}{\rho \partial x} - \frac{\partial(\rho E_t)}{\rho \partial x} - \frac{\partial(\rho E_r)}{\rho \partial x} - \frac{\partial(\rho E_v)}{\rho \partial x} - \frac{1}{4} \left(U^2 + \frac{1}{2\lambda_x} \right) \left(\frac{K_t a_4}{\lambda_t} + \frac{K_r a_5}{\lambda_r} + \frac{K_v a_6}{\lambda_v} \right) - \frac{A}{2} \left(U^2 + \frac{1}{2\lambda_x} \right) \quad (28)$$

$$a_3 = 4\lambda_x^2 [C - BU], \quad a_2 = 2\lambda_x [b_2 - b_1 U - \frac{U a_3}{\lambda_x}], \quad a_1 = A - \left(U^2 + \frac{1}{2\lambda_x} \right) a_3 - U a_2 \quad (29)$$

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CONTACT

The authors can be reached via the following email addresses: chunpei@zonatech.com; danny@zonatech.com; makxu@ust.hk .

NOMENCLATURE, ACRONYMS, ABBREVIATIONS

λ	mean free path
γ	specific heat ratio, $=C_p/C_v$
τ	relaxation time
μ	viscosity
ρ	density
λ	mean free path
ξ	internal particle velocity
Θ_v	characteristic vibrational temperature
Θ_d	characteristic dissociation temperature
f	velocity distribution function with multiple temperatures
f_{eq}	velocity distribution function with single temperature
g	equilibrium velocity distribution function
m	atomic mass
k	Boltzmann constant
p	pressure
E	energy
F	macroscopic flux
K	degree of freedom
U	mean velocity
W	macroscopic property variables
Z_r	specific rotational energy relaxation number , =3 in this paper
Z_v	specific vibrational energy relaxation number , =50 in this paper
T_n	translational temperature normal to the planar shock wave
T_t	translational temperature parallel to the planar shock wave
T_{tr}	averaged translational temperature
$T_{tr,r}$	averaged temperature calculated from translational and rotational temperature
T_v	vibrational temperature
T_{eq}	equilibrium temperature
BGK	Bhatnagar-Gross-Krook
CFD	Computational Fluid Mechanics
Kn	Knudsen number